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Key issues for accurate simulation of a-Si:H / c-Si heterojunction solar cells

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Abstract

Accurate simulation of a-Si:H / c-Si heterojunction (HET) solar cells is mandatory for acquiring a deeper understanding of device physics, better knowledge of material properties, and thus improving solar cells efficiency towards the 26% theoretical limit.
The purpose of this paper is to provide relevant guidelines and to highlight key issues for accurate and physically-based HET solar cells simulation. The need for a 2D simulation approach is demonstrated, together with an accurate description of the device optical performance. For the first time, a unified set of models and material parameters is proposed for reproducing experimental IV characteristics under illumination and obscurity conditions, considering state-of-the-art material parameters and localized defects. Finally, the key role of solar cell simulation is demonstrated for further device optimization.

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Keywords: heterojunction solar cells; amorphous Silicon; photogeneration rate; illuminated IV; dark IV

1. Introduction

Among the different technologies available for photovoltaic electricity production, amorphous / crystalline (a-Si:H / c-Si) silicon heterojunction solar cells (HET) is one of the most promising candidate for industrialization. Indeed, this technology offers two crucial advantages. First, it presents high efficiencies thanks to high open-circuit values (good passivation properties of a-Si:H combined to the

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beneficial effect of the a-Si:H / c-Si junction on the built-in voltage). Secondly, it enables production cost reduction compared to classical silicon technologies [1]. Efficiencies over 23% have been already achieved using this concept [2].

Still, at this point, further efficiency improvement doesn't appear straight-forward : an in-depth understanding of the device physics appears mandatory to pursue cell performance increase. Owing to the large number of variables (layer thicknesses, a-Si:H defects distribution, effective doping concentration, etc…), scrutinizing the effect of each variable on the overall performance of the solar cell is experimentally unfeasible. Numerical simulation using TCAD software provides a convenient way to evaluate the role of various parameters [3, 4].

This paper provides guidelines for an accurate simulation of HET solar cells. It highlights the importance of a multi-dimensional approach, and the most critical issues in both optical and electrical modeling. Finally, examples of HET devices optimization are shown, illustrating the driving role of simulation on technology improvement.

The experimental data shown in this work have been measured on a state-of-the art HET solar cell [5] fabricated at INES (French National Institute for Solar Energy), featuring ITO / a-Si:H(p) / a-Si:H(buffer) / c-Si(n) / a-Si:H(buffer) / a-Si:H(n) / ZnO layers, without texturization.

2. Importance of a multi-dimensional approach

If 1D simulations can provide useful information about conduction mechanisms, recombination losses and the optical performance of an HET solar cell, they fail to accurately model the lateral current flowlines in the semiconductor and TCO regions (see Figure 1), the voltage drop between metallization fingers and the contact shadowing. As a consequence, 1D or macroscopic models (e.g. PC1D, AFORS-HET, 2-diodes equivalent circuit [6, 7, 8]) are unable to reproduce experimental Current-Voltage (IV) characteristics in both dark and illumination conditions with a unique set of material parameters [9], as in other solar cells technologies [10, 11].

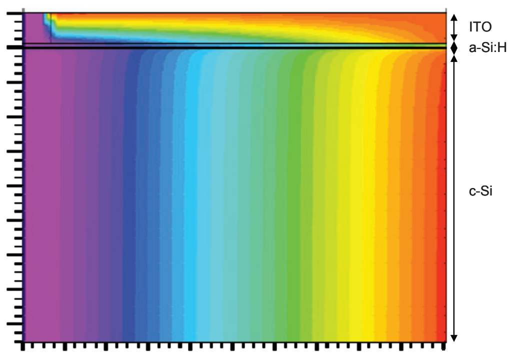


FIGURE 1. Current flowlines in a ITO / a-Si:H / c-Si HET structure. Front side contact is located on the top-left side of the structure.

As observed in Figure 2, 97% of an HET solar cell can be represented by a periodic pattern. Taking advantage of this symmetry, it is possible to strongly reduce the size of the base 2D structure and achieve a good trade-off between simulation accuracy and computational burden. The structure considered in this work is rounded by a dashed line in Figure 2. In this work, the performance of HET solar cells was investigated by using Silvaco Atlas as the numerical simulation tool, which accounts for both optical and electrical material properties and physical phenomena, and provides a wide choice of physical models for recombination losses, transport mechanisms and electrostatics.

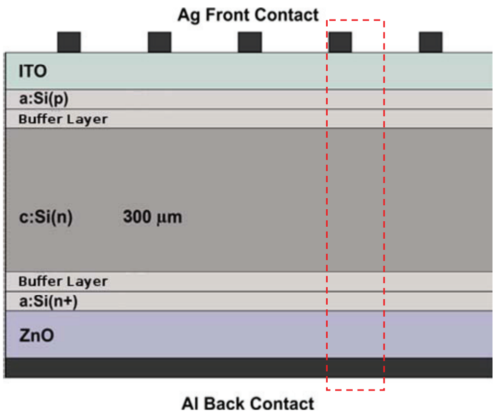


FIGURE 2. Cutline of an HET solar cell. The red dashed line rounds the 2D structure considered in this work.

3. Optical simulation of photogeneration rate

Photogeneration rate calculation is a key-issue for the accurate simulation of solar cell electrical characteristics. It describes the optical performance of the cell (reflectivity, absorbance, transmittance) and provides the quantity of photogenerated carriers in the Silicon base.

HET solar cells feature ultra-thin TCO and a-Si:H layers (a few nanometers thick). In this case, the conventional ray-tracing method [12] is no longer relevant, as it does not account for optical interferences in the ITO antireflective coating and a-Si:H layers, which thicknesses are in the order of magnitude of the incoming wavelengths. Moreover, attention must be paid to the front side contacts shadowing, and, once again, the need for a 2D optical simulation is highlighted.

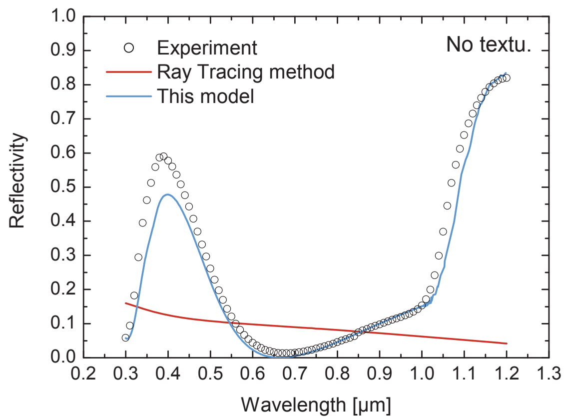


FIGURE 3. Measured reflectivity of an HET solar cell (no texturization) compared to the conventional ray-tracing method and this model (both implemented in Silvaco Atlas).

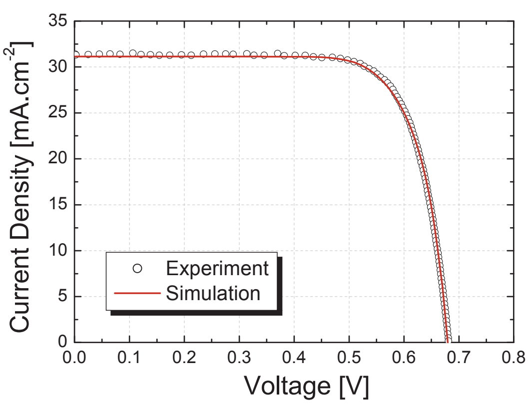
In this way, we have developed an Atlas-compatible model which accounts for both optical interferences in thin layers and contact shadowing. This method is based on the well-known transfer matrices method [13] and has been applied without any calibration parameters (material thicknesses and refractive indices (n,k) had been deduced from ellipsometry measurements). Figure 3 shows the measured reflectivity of the HET solar cell considered in this work compared to the conventional ray-tracing method and our model. An important discrepancy is observed using ray-tracing, which validates the necessity of an advanced optical modeling strategy when considering ultra-thin material layers.

4. Electrical simulation

The main difficulty in HET solar cells simulation lies in the important number of material parameters that have to be set, which depends on both process conditions and the physical models considered. An accurate description of the overall stack would require various advanced characterization techniques and a deeper understanding of the process conditions influence on material behavior. Such knowledge has not been reached yet, as illustrated by the large discrepancy of material parameters reported in the literature [14, 15, 16].

In this work, we have chosen a pragmatic approach: all the material parameters have been considered in the range of the values reported in the literature, keeping in mind that they are *effective* macroscopic parameters, unable to accurately describe stand-alone materials.

Once being confident about the computed photogeneration rate in the cell, experimental IV characteristics under AM1.5 illumination and obscurity conditions have been compared to simulation results. For the first time, we demonstrate that a unified set of physical models and material parameters is able to reproduce both illuminated and dark IV experiments, using standard material parameters and considering localized defects in the structure with an appropriate home-developed method [17].



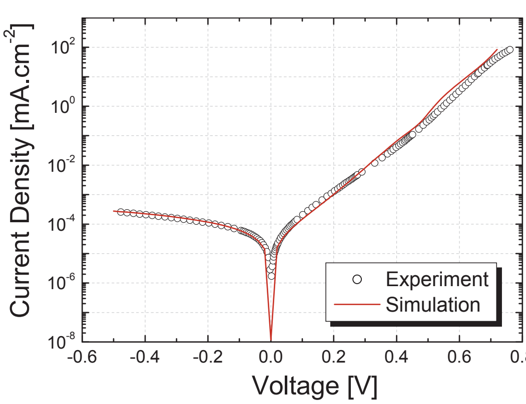


FIGURE 4. Experimental IV characteristics under illumination (left) and obscurity (right) conditions of the HET solar cell considered in this work, compared to simulation results.

a-Si:H and ITO layers have been individually and empirically optimized for years. However, the complexity of an HET solar cell structure is such that simulation is required for their overall optimization. Indeed, although considered as a second order effect a few years ago, coupling effects between layers have to be taken into account for further solar cell performance enhancement. In this way, once being calibrated on experimental results, our simulation approach allows to measure the influence of various parameters on the macroscopic behaviour of the cell, such as for example a-Si:H doping concentration, material thicknesses and interface traps concentration. For instance, Figure 5 shows the influence of either ITO, a-Si:H(p), a-Si:H(buffer), a-Si:H(n) or ZnO thicknesses on the solar cell Fill Factor (FF) and open-circuit voltage (V_{oc}). It is shown that the front side a-Si:H buffer layer thickness optimization is of prime importance for achieving a good trade-off between high V_{oc} and high FF.

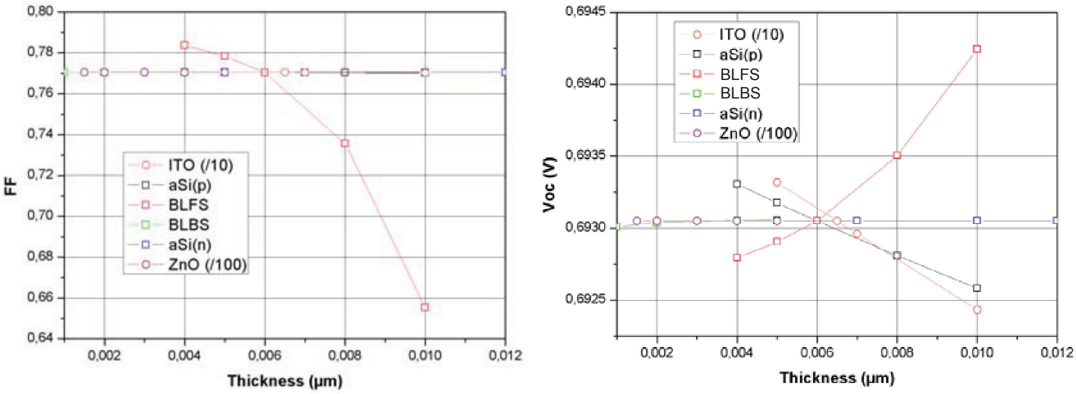


FIGURE 5. Influence of material thicknesses on the solar cell Fill Factor (left) and open-circuit voltage (right). BLFS and BLBS are the front and back side a-Si:H buffer layers, respectively.

5. Conclusion

The most important issues for accurate a-Si:H / c-Si heterojunction solar cells simulation have been highlighted. Silvaco Atlas has been demonstrated to be a relevant numerical simulation tool, as it accounts for 2D physical phenomena (contact shadowing, lateral conduction flowlines, localized defects), and for both optical and electrical material properties.

A new optical method has been implemented in Silvaco Atlas for considering both contact shadowing and optical interferences in layers as thin as the incoming wavelengths: experimental reflectivity is well reproduced by this approach, allowing a relevant simulation of the photogeneration rate and the short-circuit current.

For the first time, a unified set of physical models and material parameters allows to reproduce experimental IV characteristics in both illumination and obscurity conditions, considering only state-of-the-art material parameters. This demonstration has been achieved thanks to the advanced modeling strategy for photogeneration rate calculation and the consideration of 2D effects and localized defects in the HET solar cell.

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